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Direct numerical simulation of effective drag in dense gas–liquid–solid three-phase flows

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ABSTRACT

Gas–liquid–solid three phase flows are commonly found in (bio-)chemical processes, e.g. in bubble slurry columns in the Fischer–Tropsch process. In order to facilitate the rational scale-up and the design of such columns, a detailed understanding of the complex phase interactions is required. In this work, we focus on the effective drag acting on particles and bubbles, using Direct Numerical Simulations. We combined the Front Tracking method of Roghair et al. (2013b) and the second order implicit Immersed Boundary method of Deen et al. (2012). The resulting hybrid Front Tracking Immersed Boundary method is able to simulate dense three phase flows and is used to study swarm effects in terms of drag. A correlation has been obtained for the drag coefficient for a system consisting of 2 mm bubbles and 1 mm particles at several phase volume fractions. In future research, the developed methodology can be applied to study the effect of the bubble and particle size and their ratio.

1. Introduction

The interest in Fischer–Tropsch processes for the production of synthetic fuels, methanol synthesis and other gas-to-liquid processes is growing in recent years, due to the increase in the oil prices. Usually these processes are performed in slurry bubble columns. To improve the design and the scale-up of these processes, fundamental understanding of the hydrodynamics and the complex three-phase interactions is required (Kantarci et al., 2005; Wang et al., 2007; Yang et al., 2007; Pan et al., 2016).

When particles are introduced to the liquid phase, the bubbles size decreases and the void fraction increases. Moreover, an increase in the solids volume fraction will also reduce the bubble rise velocity (Kantarci et al., 2005; Wang et al., 2007; Hooshyar et al., 2013; Baltussen et al., 2013; Pan et al., 2016). Hooshyar et al. (2013) studied the mechanism of this decrease of the bubble rise velocity for neutrally buoyant particles. The mechanism depends on the Stokes relaxation time of the particles. For particles with a relatively small relaxation time, the particles only influence the bubble rise velocity via an increase of the apparent viscosity. Although larger particles will also influence the apparent viscosity, the decrease in the bubble rise velocity is mainly caused by the collisions of the particles with the bubbles.

To improve our predictive capabilities, a more fundamental understanding of the effect of the particles on the bubble rise velocity and the effect of the bubbles on the particle velocities is needed. Because of the experimental limitations in terms of optical access and intrusiveness, Multiphase Computational Fluid Dynamics (MCFD) is an attractive tool to study these effects. Typically, industrial size bubble slurry columns are tens of meters tall, while the bubbles and the particles are in the order of millimeters and tens of micrometers, respectively. Because of these different length scales and associated time scales, MCFD is not suited to fully resolve all relevant details using a single model. To overcome this problem, a multi-scale modeling approach is adapted. In this approach, the smaller scale models provide closures for the larger scale models, ensuring accurate representation of the small scale phenomena while using relatively modest computational power (van Sint Annaland et al., 2003; Deen et al., 2004; Yang et al., 2007; Raessi et al., 2010; Roghair et al., 2011; Baltussen et al., 2013; Pan

Abbreviations: *b*, Bubble; *B*, Buoyancy; *c*, Central; *col*, Due to particle-particle collisions; *D*, Drag; DNS, Direct Numerical Simulations; Eo, Eötvös number, $g_z d_b^2 \Delta\rho/\sigma$; FT, Front Tracking; *g*, Gas phase; IB, Immersed Boundary; *l*, Liquid phase; *nb*, Neighboring; MCFD, Multiphase Computational Fluid Dynamics; Mo, Morton number, $g_z \mu_l^4 \Delta\rho/(\rho_l^2 \sigma^3)$; *P*, Pressure; *rel*, Relative; Re, Reynolds number, $\rho|\mathbf{v}|d_b/\mu_l$; *s*, Solid phase; *z*, Direction of the gravitation; σ, Surface tension; ∞, Single bubble or particle infinite liquid

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Nomenclature

Roman symbol

a, b, C	Coefficient
d	Diameter (m)
$\mathbf{F}$	Force density or Force (N/m^3 or N)
$\mathbf{g}$	Gravity acceleration (m/s^2)
I	Moment of inertia (Kg·m^2)
$\mathbf{n}$	Normal
p	Pressure (Pa)
t	Time (s)
$\mathbf{r}$	Distance (m)
$\mathbf{u}$	Liquid, fluid velocity (m/s)
$\mathbf{v}$	Bubble velocity (m/s)
V	Volume (m^3)
$\mathbf{w}$	Particle velocity (m/s)Greek symbols
α	Void fraction
μ	Viscosity (Pa·s)
ρ	Density (kg/m^3)
σ	Surface tension coefficient (N/m)
τ	Stress tensor (Pa)
ϕ	Solid volume fraction
ψ	Velocity component (m/s)
ω	Rotational velocity (1/s)

et al., 2016).

1.1. Multiscale modeling

In the multi-scale modeling approach, the largest scales are simulated using Euler–Euler models. These models consider all phases as continuous interpenetrating fluids, which enables in principle the simulation of an industrial size bubble column. However, these models require closure relations to accurately capture the bubble-bubble, bubble-liquid, bubble-particle, liquid-particle and particle-particle interactions (Yang et al., 2007; Roghair et al., 2011; Baltussen et al., 2013; Pan et al., 2016).

These closures can be assessed and tested using Euler–Lagrangian models, which are the intermediate scale models of the multi-scale modeling approach. In Euler–Lagrangian models, the volume-averaged Navier–Stokes equations are solved for the continuous phase, while the bubbles and the particles are tracked as Lagrangian particles. Although the large scale swarm effects and the effects of coalescence and break-up can be studied adequately using these models, the models only solve the volume-averaged Navier–Stokes equations and do not resolve the dynamics of the dispersed elements (bubbles and/or particles). Therefore closures still have to be included for the bubble-liquid and particle-liquid interactions, e.g. drag and lift correlations (Deen et al., 2004; Yang et al., 2007; Roghair et al., 2011; Baltussen et al., 2013; Pan et al., 2016).

These correlations for the bubble-liquid and particle-liquid interactions can be generated using the smallest scale models: Direct Numerical Simulations (DNS). In DNS, all details of the flow field are fully resolved, i.e. the governing equations are solved without any rigorous a priori assumptions or simplifications. This leads to a very accurate description of the flow field, but limits the simulations to $O(10^2)$ bubbles due to the high computational costs (Deen et al., 2004; Yang et al., 2007; Roghair et al., 2011; Baltussen et al., 2013).

1.2. Objectives

In this work, dense gas–liquid–solid three-phase flows will be studied using DNS. Three-phase DNS methods have been developed by several authors starting from the available two-phase methods. Li et al. (2001) combined the Euler–Lagrange approach with a DNS method. Although this method is able to study three phase flows, closures are still required for the solid–liquid interactions, because the particles are taken into account as Lagrangian point particles. Ge and Fan (2006), Jain et al. (2012) and Baltussen et al. (2016) combined a front capturing technique to capture the gas–liquid interface and an Immersed Boundary (IB) method to implement the no-slip boundary condition. These front capturing techniques reconstruct the interface instead of directly tracking the interface. Although these models inherently allow for break-up and coalescence, the obtained break-up and merging of the bubbles might be unphysical. Therefore, Deen et al. (2009) and Baltussen et al. (2013) combined a front tracking technique with an IB method. In these models, coalescence and break-up of bubbles does not take place, unless it is included via a sub-grid model.

In this work, dense gravity driven particle/bubble swarms will be studied. To ensure a constant bubble size and to prevent unphysical merging of the bubbles, the gas–liquid interface is described using the Front Tracking (FT) method of Roghair et al. (2013a). The particle-fluid interaction is described using the second order implicit IB method of Deen et al. (2012), because this method does not require an effective particle diameter.

This paper is organized as follows. First of all, an explanation of the applied numerical method is given. Subsequently, the simulation settings will be discussed whereafter the effect of the void fraction and the solids volume fraction on the drag coefficient of the bubbles and the particles will be presented and discussed.

2. Numerical method

The used three phase DNS method is a combination of the FT method of Roghair et al. (2013a) and the second order IB method of Deen et al. (2012). This paper contains only a brief discussion of both methods, particularly focusing on the combination of both methods and the modification required to enable the calculation of three-phase systems. The combined FT-IB model solves the continuity equation, Eq. (1), and the Navier–Stokes equations, Eq. (2), assuming incompressible flow:

$$\nabla\cdot\mathbf{u} = 0 \tag{1}$$

$$\rho\frac{\partial\mathbf{u}}{\partial t} = -\nabla p - \rho\nabla\cdot(\mathbf{uu}) - \nabla\cdot\tau + \rho\mathbf{g} + \mathbf{F}_\sigma \tag{2}$$

Because the velocity field is continuous across the gas–liquid interface, the Navier–Stokes equations can be solved using an one-field approximation. The used viscosity in all grid cells is the volume averaged viscosity. At a three phase interface, the viscosity of the particle phase is set equal to the liquid viscosity. The surface tension at the gas–liquid interface is taken into account by an extra force density, $\mathbf{F}_\sigma$, which is introduced near the interface. This force density is calculated using the triangular markers, that represent the gas–liquid interface. Each marker is subject to tensile forces exerted by the three neighboring markers. The summation of these tensile forces gives the surface force exerted on the marker, which is mapped to the surrounding cells using a mass-weighing function (Dijkhuizen et al., 2010b; Roghair, 2012). To alleviate the difference, due to the mismatch between the discretisation of the surface tension and the pressure field, the surface tension calculations is augmented with the so-called “pressure-jump correction” (Renardy and Renardy, 2002; Francois et al., 2006; Dijkhuizen et al., 2010b), leading to less parasitic currents.

The no-slip boundary condition at the particle surface is taken into account implicitly at the level of the discretised Navier–Stokes equations. At this level, each velocity component at a certain node in the fluid, ψ_c, can be described as a function of the velocity components of the neighboring nodes, ψ_{nb}, with Eq. (3).